Non-singular dislocation loops in gradient elasticity

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Abstract

Using gradient elasticity, we give in this Letter the non-singular fields produced by arbitrary dislocation loops in isotropic media. We present the 'modified' Mura, Peach-Koehler and Burgers formulae in the framework of gradient elasticity theory.

Keywords: dislocation loops; gradient elasticity.

We investigate the general theory of curved dislocations in isotropic media. This topic is important in nano-mechanics of dislocations and can be found in any standard book on dislocation theory using the classical theory of elastostatics [1, 2, 3, 4, 5]. The key-formulae in the 'classical theory' of a closed dislocation loop L are the Mura formula for the elastic distortion tensor

$$\beta^0_{ij}(\boldsymbol{x}) = -\frac{b_k}{8\pi}\oint_L \Big[\big(\epsilon_{jkl}\delta_{ir} - \epsilon_{rkl}\delta_{ij} + \epsilon_{rij}\delta_{kl}\big)\partial_l\Delta + \frac{1}{1-\nu}\,\epsilon_{rkl}\partial_l\partial_i\partial_j\Big] R\,\mathrm{d}L'_r\,, \tag{1}$$

the Peach-Koehler formula for the stress tensor

$$\sigma^0_{ij}(\boldsymbol{x}) = -\frac{\mu b_k}{8\pi}\oint_L \Big[\big(\epsilon_{jkl}\delta_{ir} + \epsilon_{ikl}\delta_{jr}\big)\partial_l\Delta + \frac{2}{1-\nu}\,\epsilon_{rkl}\big(\partial_i\partial_j - \delta_{ij}\Delta\big)\partial_l\Big] R\,\mathrm{d}L'_r \tag{2}$$

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and the Burgers formula for the displacement vector

$$u_i^0(\boldsymbol{x}) = \frac{b_i}{8\pi}\int_S \Delta\partial_j R\, \underset{\cdot}{\mathrm{S}}'_j + \frac{b_l\epsilon_{rlj}}{8\pi}\oint_L \left\{\delta_{ij}\Delta - \frac{1}{1-\nu}\,\partial_i\partial_j\right\} R\, \underset{\cdot}{\mathrm{L}}'_r\,, \tag{3}$$

where $R = |\boldsymbol{x}-\boldsymbol{x}'|$, μ is the shear modulus, ν is Poisson's ratio, b_i is the Burgers vector of the dislocation line element $\underset{\cdot}{\mathrm{L}}'_r$ at $\boldsymbol{x}'$ and $\underset{\cdot}{\mathrm{S}}'_j$ is the dislocation loop area. The surface S is the dislocation surface which is a cap of the dislocation line L. These equations give the elastic fields and the displacement produced by a dislocation loop in isotropic media. They are valid only in the far-field due to singularities based on the unphysical description of the dislocation core as singular delta functions. The purpose of this Letter is to give straightforward expressions for the dislocation fields which are free from singularities

A straightforward framework to obtain non-singular fields of dislocations is the so-called theory of gradient elasticity. Particularly in a simplified, robust and often-used strain gradient elasticity called gradient elasticity of Helmholtz type the strain energy density has the form [6, 7]

$$W = \frac{1}{2}\,C_{ijkl}\beta_{ij}\beta_{kl} + \frac{1}{2}\,\ell^2 C_{ijkl}\partial_m\beta_{ij}\partial_m\beta_{kl}\,, \tag{4}$$

where C_{ijkl} is the tensor of elastic moduli, $\beta_{ij} = \partial_j u_i - \beta^{\mathrm{P}}_{ij}$ is the elastic distortion tensor, u_i and β^{P}_{ij} denote the displacement vector and the plastic distortion tensor respectively and ℓ is the material length scale parameter of gradient elasticity. For dislocations, ℓ is related to the dislocation core radius. Gradient elasticity is a continuum model of dislocations with core spreading. Non-singular fields of straight dislocations were obtained in the framework of gradient elasticity of Helmholtz type by Gutkin and Aifantis [8], Lazar and Maugin [6, 9] and Gutkin [10]. Surprisingly, not a single work has been done up to now in the direction of non-singular dislocation loops using strain gradient elasticity theory. The reason lies probably in the expected mathematical complexity of the problem.

For an isotropic material the tensor of elastic moduli reduces to

$$C_{ijkl} = \mu\Big(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} + \frac{2\nu}{1-2\nu}\,\delta_{ij}\delta_{kl}\Big)\,. \tag{5}$$

As shown by Lazar and Maugin [6, 9] the following governing equations for the displacement vector and the elastic distortion tensor can be derived from the framework of gradient elasticity of Helmholtz type

$$L\, u_i = u_i^0\,, \tag{6}$$
$$L\, \beta_{ij} = \beta_{ij}^0\,, \tag{7}$$

where $L = 1 - \ell^2\Delta$ is the Helmholtz operator. The singular fields u_i^0 and β^0_{ij} are the sources in the inhomogeneous Helmholtz equations (6) and (7). The Helmholtz equations (6) and (7) can be further reduced to inhomogeneous Helmholtz-Navier equations

$$L\, L_{ik}u_k = C_{ijkl}\partial_j\beta^{\mathrm{P},0}_{kl}\,, \tag{8}$$
$$L\, L_{ik}\beta_{km} = -C_{ijkl}\epsilon_{mlr}\partial_j\alpha^0_{kr}\,, \tag{9}$$

where $L_{ik} = C_{ijkl}\partial_j\partial_l$ is the differential operator of the Navier equation. In Eqs. (8) and (9) the source terms are now the plastic distortion $\beta^{\mathrm{P},0}_{kl}$ and the dislocation density α^0_{kr} known from classical elasticity. For a dislocation loop, they read [11]

$$\alpha^0_{ij} = b_i\,\delta_j(L) = b_i \oint_L \delta(\boldsymbol{x}-\boldsymbol{x}')\,\mathrm{d}L'_j\,, \tag{10}$$

$$\beta^{\mathrm{P},0}_{ij} = -b_i\,\delta_j(S) = -b_i \int_S \delta(\boldsymbol{x}-\boldsymbol{x}')\,\mathrm{d}S'_j\,. \tag{11}$$

The corresponding three-dimensional Green tensor of the Helmholtz-Navier equation is defined by

$$L\,L_{ik}\,G_{kj} = -\delta_{ij}\,\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{12}$$

and is calculated as

$$G_{ij}(R) = \frac{1}{16\pi\mu(1-\nu)}\Big[2(1-\nu)\delta_{ij}\Delta - \partial_i\partial_j\Big]A(R)\,. \tag{13}$$

Hence

$$A(R) = R + \frac{2\ell^2}{R}\Big(1-\mathrm{e}^{-R/\ell}\Big)\,. \tag{14}$$

In the limit $\ell \to 0$, the three-dimensional Green tensor of classical elasticity [4, 5] is recovered in Eqs. (13) and (14).

Using the Green tensor (13) and after a straightforward calculation all the generalizations of the key-formulae (1)–(3) to gradient elasticity are obtained. The non-singular elastic distortion of a dislocation loop is given by

$$\beta_{ij}(\boldsymbol{x}) = -\frac{b_k}{8\pi}\oint_L \Big[\big(\epsilon_{jkl}\delta_{ir} - \epsilon_{rkl}\delta_{ij} + \epsilon_{rij}\delta_{kl}\big)\partial_l\Delta + \frac{1}{1-\nu}\,\epsilon_{rkl}\partial_l\partial_i\partial_j\Big]A(R)\,\mathrm{d}L'_r\,. \tag{15}$$

This is the 'Mura formula' for a dislocation loop in gradient elasticity. Using the constitutive relation $\sigma_{ij} = C_{ijkl}\beta_{kl}$, we find the non-singular stress field produced by a dislocation loop

$$\sigma_{ij}(\boldsymbol{x}) = -\frac{\mu b_k}{8\pi}\oint_L \Big[\big(\epsilon_{jkl}\delta_{ir} + \epsilon_{ikl}\delta_{jr}\big)\partial_l\Delta + \frac{2}{1-\nu}\,\epsilon_{rkl}\big(\partial_i\partial_j - \delta_{ij}\Delta\big)\partial_l\Big]A(R)\,\mathrm{d}L'_r\,, \tag{16}$$

which can be interpreted as the Peach-Koehler formula within the framework of gradient elasticity. The key-formula for the non-singular displacement vector in gradient elasticity is obtained as

$$u_i(\boldsymbol{x}) = \frac{b_i}{8\pi}\int_S \Delta\partial_j A(R)\,\mathrm{d}S'_j + \frac{b_l\epsilon_{rlj}}{8\pi}\oint_L \Big\{\delta_{ij}\Delta - \frac{1}{1-\nu}\,\partial_i\partial_j\Big\}A(R)\,\mathrm{d}L'_r\,, \tag{17}$$

which is the Burgers formula in the framework of gradient elasticity of Helmholtz type. Eq. (17) determines the displacement field of a single dislocation loop. The Eqs. (15)–(17) are straightforward, simple and closely resemble the singular solutions of classical elasticity

theory. In the limit $\ell \to 0$, the classical expressions (1)–(3) are recovered from Eqs. (15)–(17). The expressions (15)–(17) retain most of the analytic structure of the classical Mura, Peach-Koehler and Burgers formulae. It is obvious that the expressions (15)–(17) are given in terms of the elementary function $A(R)$ shown in Eq. (14) instead of the classical expression R. The simplicity of our results is based on the use of gradient elasticity theory of Helmholtz type. Our results can be used in computer simulations of dislocation cores at nano-scale and in numerics of dislocation dynamics like fast numerical sums of the relevant fields as used for the classical equations (e.g. [12, 5]). They may be implemented in dislocation dynamics codes (finite element implementation) and compared to atomistic models.

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